Entanglement perturbation theory for the elementary excitation in one dimension

Sung Gong Chung and Lihua Wang

Department of Physics and Nanotechnology Research and Computation Center,
Western Michigan University, Kalamazoo, MI 49008-5252, USA

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The entanglement perturbation theory is developed to calculate the excitation spectrum in one dimension. Applied to the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model, it reproduces the des Cloiseaux-Pearson Bethe ansatz result. As for spin-1, the spin-triplet magnon spectrum has been determined for the first time for the entire Brillouin zone, including the Haldane gap at $k = \pi$.

The importance of elementary excitations in condensed matter systems may be best understood in the superfluid ^{4}He. The Tisza two-fluid model with the experimentally found phonon-roton spectrum explains fundamental properties of the superfluid ^{4}He [1]. Feynman's effort then to explain the roton spectrum is well known [2]. From the theorem of Bloch-Floquet, the elementary excitation with momentum k for a translationally invariant Hamiltonian H is written as

$$\Psi_k = \sum_{l=1}^{N} e^{ikl} O_l^\dagger |g\rangle \tag{1}$$

where $|g\rangle$ is the ground state and the summation over l extends over the entire lattice sites. The O_l is a local cluster operator to be determined for a given Hamiltonian.

In spite of a simplicity and validity of the expression (1), not much progress has been made along this line since the days of Feynman. The Heisenberg antiferromagnet (HA) described by the Hamiltonian

$$H = J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tag{2}$$

is probably the best studied system concerning the excitation spectrum. In particular, Haldane conjectured in 1983 that the half-odd integer and integer spins might behave essentially differently [3], which together with a field theoretic prediction of Affleck [4] for a logarithmic correction to the power-law behavior in the spin-spin correlation function in the spin-$\frac{1}{2}$ case, triggered an intensive study of HA ranging from the exact diagonalization [5, 6] and Monte Carlo [7, 8] to DMRG (density matrix renormalization group) [9–11]. These studies along with the Bethe ansatz solution for the spin-$\frac{1}{2}$ case [12] lead to a confirmation of the both claims. Concerning the elementary excitation for the entire Brillouin zone, however, Takahashi's two attempts following the Feynman variational method for ^{4}He and a projector-Monte Carlo method were the only studies [13, 14]. And none of the previous studies gave a serious consideration to the expression (1).

In this Letter, we analyze (1) exactly for the HA (2) with periodic boundary conditions by the recently developed entanglement perturbation theory (EPT). EPT is a novel many-body method which takes into account correlations systematically. Its mathematical implementation is singular value decomposition (SVD), intuitively *divide and conquer*. EPT has addressed so far classical statistical mechanics [15], 1D quantum ground states [16] and 2D quantum ground states [17]. We here address the elementary excitation in one dimension. By EPT, we are not only free from a negative sign problem which is inherent to MC for quantum spins and fermions, but can also handle an order of magnitude larger systems than MC and DMRG. The key of the success lies in our ability of calculating the ground state $|g\rangle$ precisely and most importantly in an *un-renormalized* form. We examine the cluster excitation operator O_l systematically. We have found that the size of the magnon is 4 lattices long at largest for both spin-$\frac{1}{2}$ and spin-1.

We solve the problem (1) in two steps. First, we find the ground state. We can do this in two ways. Either to consider the density matrix eigenvalue problem $e^{-\beta H}|g\rangle = e^{-\beta E_g}|g\rangle$ with $\beta \to 0$ as done in [16] (EPT-g1). There, the density matrix is expressed in a matrix, tensor product form, reducing the problem to that of the partition function calculation in the 2D, 3D Ising model [15]. This method is particularly suited to study the infinite system because then we only need to consider the largest eigenvalue. Or to directly minimize the energy $\langle g|H|g\rangle / \langle g|g\rangle$ as formulated in [17] (EPT-g2). The second method is free from the parameter β, but it needs to handle a number of eigenvalues no matter how large the system size. Either way, the starting wave function is that of SVD-ed one [15–17],

$$|g\rangle = \cdots \zeta_{\alpha\beta}^1(s_1) \zeta_{\beta\gamma}^2(s_2) \zeta_{\gamma\delta}^1(s_3) \cdots \tag{3}$$

on the basis $\cdots |s_1\rangle \otimes |s_2\rangle \otimes |s_3\rangle \otimes \cdots$ where $|s_i\rangle$ denotes spin states on the site i, and the local bi-partite wave functions $\zeta^{1,2}$ reflect the local antiferromagnetic interaction.

Let us consider the variational problem, EPT-g2,

$$\delta E_g = \delta \frac{\langle g|H|g\rangle}{\langle g|g\rangle} = 0 \tag{4}$$
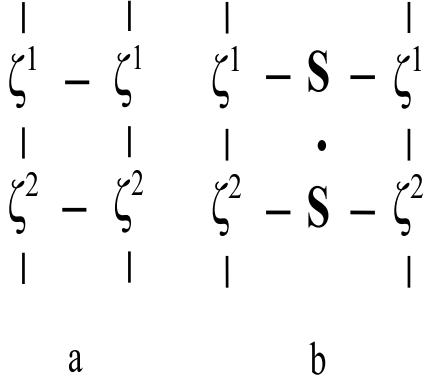
FIG. 1: (a) Matrix A. The vertical lines denote entanglement while the horizontal ones the basis spin states. The upper 2 external verticle lines constitute the right index of A while the lower 2 the left index. The inner lines should be contracted. (b) Matrix $\hat{A}$

with respect to $\zeta^{1,2}$. First consider $\delta\langle g|g\rangle$. For the periodic ring of N bi-lattice units, we have

$$\langle g|g\rangle = T_r A^N \tag{5}$$

with the matrix A shown in Fig.1a. The variation with respect to $\zeta^{1,2}$ is, due to the translational symmetry, N times the variation of $\zeta^{1,2}$ at a particular bi-lattice unit. The idea is to use an initial trial for $\zeta^{1,2}$ and evaluate the trace over the $N-1$ bi-lattice units, which can be done as follows. Writing the left and right eigenvector matrixes as L and R and the diagonal eigenvalue matrix as σ, the matrix A is written as

$$A = R\sigma\tilde{L} \tag{6}$$

where $\tilde{L}$ is the transpose of L, with the property $\tilde{L}\cdot R = 1$. We can thus write

$$\langle g|g\rangle = \sum_i \sigma_i^{N-1}\tilde{L}_i A R_i \tag{7}$$

Now note that the last form (7) contains $\zeta^{1,2}$ quadratically, thus written as either $\tilde{\zeta}^1 M^1(\zeta)\zeta^1$ or $\tilde{\zeta}^2 M^2(\zeta)\zeta^2$ with

$$M^1(\zeta)_{l,r} = \delta_{ls,rs}\sigma_i^{N-1}L_i(lt,rt)R_i(lu,ru)$$
$$\zeta_{ld,lt}^2(ts)\zeta_{rd,rt}^2(ts) \tag{8}$$

where the indexes are put together as $l = (lu-1)\cdot p\cdot n_s + (ld-1)\cdot n_s + ls$ and $r = (ru-1)\cdot p\cdot n_s + (rd-1)\cdot n_s + rs$ where p denotes the entanglement size and n_s the local spin degrees of freedom, and summations are implied for the repeated indexes. And likewise for $M^2(\zeta)$. As for the numerator $\langle g|H|g\rangle$, because of the translational symmetry, the variation with respect to $\zeta^{1,2}$ is again N times the variation of $\zeta^{1,2}$ at a particular bi-lattice unit. Since the Hamiltonian is a sum of local nearest neighbor interactions, a typical term in $\langle g|H|g\rangle$

size	EPT	BA
16	-0.4463935	-0.4463935
64	-0.4433459	-0.4433485
256	-0.4431555	-0.4431597

TABLE I: Comparison of the ground state energies between BA and EPT with the entanglement $p = 15$ for 16 spins, 22 for 64 and 36 for 256

distance	EPT	BA
1	-0.1477187	-0.1477157
2	0.0606790	0.0606798
3	-0.0502424	-0.0502486
4	0.0346217	0.0346528
5	-0.0308335	-0.0308904
6	0.0243932	0.0244467
7	-0.0224726	-0.0224982

TABLE II: Comparison of G^z over the first 7 sites between BA and EPT with $p = 36$ for 256 spins

is $\tilde{L}_j A R_i \sigma_j^{l-2}\tilde{L}_i \hat{A} R_j \sigma_i^{N-l}$ where $\hat{A}$ is given by Fig.1b. A summation is carried out over the terms containing $\zeta^{1,2}$ except a quadratic term to be variated, and $\langle g|H|g\rangle$ can be written as either $\tilde{\zeta}^1 N^1(\zeta)\zeta^1$ or $\tilde{\zeta}^2 N^2(\zeta)\zeta^2$. Thus the variational problem (4) leads to nonlinear, generalized eigenvalue problems

$$M^i(\zeta)\zeta^i = E_g N^i(\zeta)\zeta^i \quad ; \quad i = 1,2 \tag{9}$$

We have solved (9) iteratively for both spin-$\frac{1}{2}$ and spin-1 for the system size up to 1024 and the entanglement size up to 38. A thorough discussion of the EPT result for the ground state properties of the xxz model with the Ising anisotropy coupling $\lambda = 0 \sim \infty$ will be given in a future publication [18]. We here concentrate on the isotropic xxx case. A convergence in the ground state energy per site occurs typically around p=20.

For spin-$\frac{1}{2}$, the exact result is given by Bethe ansatz (BA) [19]. The ground state energies per site for 16, 64 and 256 spins by EPT and BA are compared in Table I. The spin-spin correlation function $G^z(l) = \langle S_z(0)S_z(l)\rangle$ is also known by BA up to lattice separations 7. Comparison of BA and EPT for 256 spins is given in Table II. As for a longer distance $l \gg 1$, an asymptotic formula is given by field theory [4]. Extensive finite size analysis with exact diagonalization, Monte Carlo and DMRG [6, 7, 11] have been done concerning the field theoretic prediction of the logarithmic correction of the form $\propto \sqrt{ln(l)}/l$ at large distance. The lattice size at which the asymptotic formula is realized is estimated to be several thousands. Fig.2 shows the EPT result of the correlation function for the spin-$\frac{1}{2}$ with 256 spins which is a lot longer than previously studied. Note that the
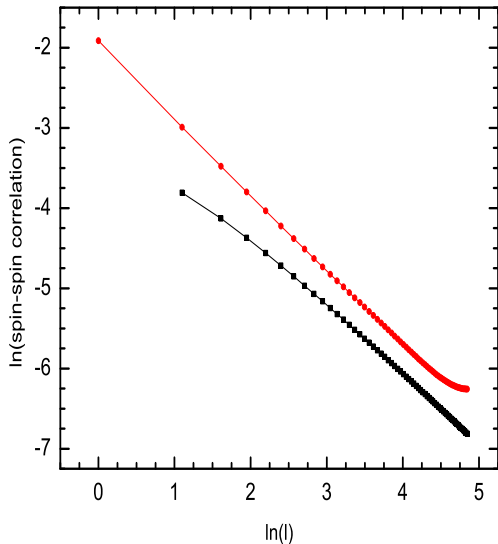
FIG. 2: Log-log plot of the spin-spin correlation function for 256 spins for spin-$\frac{1}{2}$. The upper line is the converged result for entanglement 32, while the lower line is the asymptotic formula from field theory.

converged and hence exact result at $p = 32$ is well fitted by a straight line, except near the central part at $l = 128$ reflecting the periodic boundary condition,

$$G^z(l) \propto l^{-0.92} \qquad (10)$$

While the greater than -1 exponent reflects the logarithmic correction, a large discrepancy between the EPT and the field theoretic asymptotic form, FT in Fig.2, for a distance $l \sim 100$ is consistent with the argument that the FT asymptotic form is correct for distances as large as several thousands. It should be noted that EPT can handle any system size, but for a larger system, a larger entanglement is necessary to get a good ground state. An interesting question then is, to calculate the correlation functions correctly for thousands-long distances, how large the entanglement p should be? In fact the issue is closely related to another field theoretic prediction [4] that the correlation functions at large distance should have a singular dependence on the Ising anisotropy parameter λ, namely $G^z = G^x$ at $\lambda = 1$ but $G^z = 4G^x$ when λ approaches 1 from below. Following the successful EPT analysis of such symmetry breaking in the 2D, 3D Ising models [15], a calculation is currently underway and will be reported elsewhere.

As for spin-1, EPT agrees with DMRG, e.g. the ground state energy per site for $N = 48$ is -1.401482 (EPT with $p = 24$) vs -1.401484 (DMRG [9]), and the spin-spin correlation function shows an exponential decay as expected for a gapped system.

An important note on the ground state algorithms EPT-g1,2 is that they can also calculate some excited states. For example, we have applied EPT-g2 to spin-1 to get the energy gap at $k = \pi$ correctly, 0.4124 (EPT with $p = 20$) vs 0.4123 (DMRG [9]) for 48 spins.

We now come to the second step, the implementation of the variational program for the elementary excitation (EPT-e),

$$\delta E_k = \delta \frac{\langle \Psi_k | H | \Psi_k \rangle}{\langle \Psi_k | \Psi_k \rangle} = 0 \qquad (11)$$

Using (1), we first rewrite E_k as

$$\varepsilon(k) = E_k - E_g = \sum_{l=1}^{2N} e^{-ikl} \frac{\langle g | O_l [H, O_0^\dagger] | g \rangle}{\langle \Psi_k | \Psi_k \rangle} \qquad (12)$$

where $[\cdots]$ means a commutator and we have used the fact that $H|g\rangle = E_g|g\rangle$, and therefore the accurate ground state wave function is a crucial ingredient in this method. Note that N is the number of bi-lattice units and $2N$ is the total number of spins. More importantly, we need the *un-renormalized* ground state which may not be easy to obtain by DMRG without an efficient restoration of the un-renormalized ground state at the end of the calculation, particularly for large systems such as 512 and 1024 spins as studied by EPT.

To carry out the variation $\delta\varepsilon(k) = 0$ with respect to the cluster operator O_l, the simplest case is the one which acts only on one site and, say, for the spin-triplet excitation, then it is uniquely $S^+ = S_x + iS_y$ for spin-$\frac{1}{2}$. In the spin-1 case, there are only two such operators, $\mu_1 = S^+$ and $\mu_2 = S^+ S_z$. The cluster operator can then be written as a linear combination $O_l = c_1\mu_1 + c_2\mu_2$ and the variation is with respect to the vector $\tilde{x} = (c_1, c_2)$, leading to a generalized eigenvalue problem

$$Tx = \varepsilon(k)Ux \qquad (13)$$

where T and U are 2×2 matrixes. The n-cluster operator O_l is generally written as a linear combination of operator products of n $n_s \times n_s$ local operators, where $n_s = 2$ for spin-$\frac{1}{2}$ and 3 for spin-1. With the increase of the cluster size of O_l, the matrix size of T and U increases like 1,4,15 and 56 (spin-$\frac{1}{2}$) and 2,16,126 and 1016 (spin-1) for the spin-triplet excitation. For example, for $n = 2$ and spin-$\frac{1}{2}$, O_l is a linear combination of the 4 local excitation operators, $S^+ \otimes 1$, $S^+ \otimes S_z$, $1 \otimes S^+$ and $S_z \otimes S^+$. The calculation of the matrixes T and U are essentially the same as in the ground state, although due to the *cluster* nature of the operator O_l and the presence of the commutator $[H, O_0^\dagger]$, we have a little lengthy algebraic procedure, details to be presented elsewhere.

Fig.3 shows the spin-triplet excitation spectrum for spin-$\frac{1}{2}$ with the chain size 512 and the cluster size n up to 4. The EPT calculation almost converged at $n = 4$, and gives an agreement of 1% precision with BA [12].
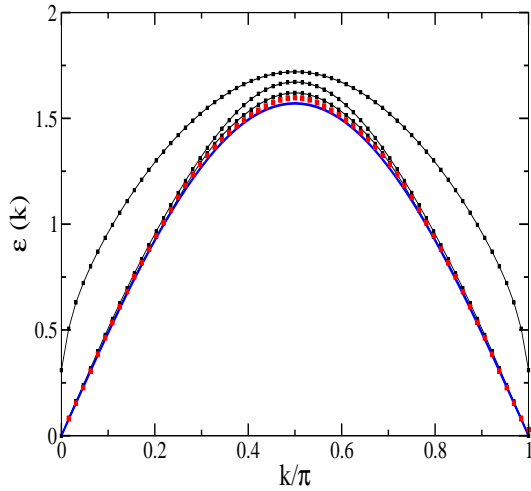
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FIG. 3: Spin triplet excitation spectrum for spin-$\frac{1}{2}$ for 512 spins. The ground state used is from p=20. From top to bottom, the cluster size is 1 to 4 (red online). The thick line (blue online) is the Bethe ansatz result [12].
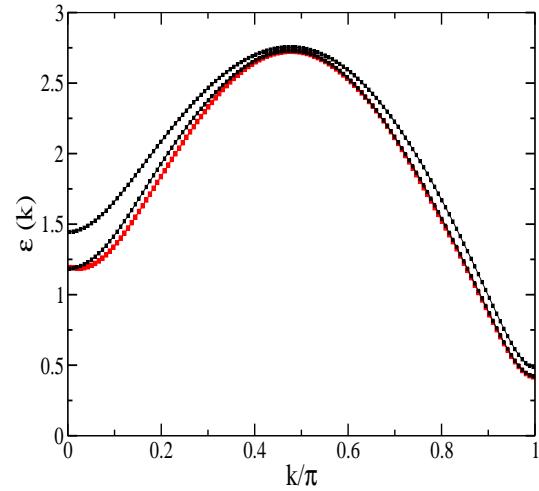

FIG. 4: Spin triplet excitation spectrum for spin-1 for 512 spins. The ground state used is from p=24. From top to bottom, the cluster size is 1 to 3 (red online).

Fig.4 shows the same for spin-1 up to the cluster size $n = 3$ where the calculation almost converged. The Haldane gap at $k = \pi$ is found by EPT to be 0.414 agreeing with the previous results [8, 10, 13]. As for the region $0 \leqslant k/\pi \leqslant 1/2$, the spin-triplet spectrum is believed to be embedded in a continuum spectrum of a pair of magnons with the total spin-z component to be 0 [20]. The exact diagonalization for $N = 14$ indeed tells us that the lowest excitation at $k = 0$ is spin singlet, presumably a $(-\pi, \pi)$ pair of spin-triplet magnons from $k = \pm\pi$ [5, 13]. We believe that the spin-triplet magnon spectrum for spin-1 for the entire Brillouin zone has been determined for the first time by EPT. Moreover EPT can handle not only the lowest but the entire spin-triplet sectors, and can be repeated for other excitations such as spin-singlet. It simply amounts to calculating not just the minimum but all the eigenvalues of (13). Such entire excitation spectra have been known only for the isotropic spin-$\frac{1}{2}$ case by Bethe ansatz, see Fig.4, 5 in [19].

In conclusion, we have developed EPT for the elementary excitation (1), where the *un-renormalized* ground state $|g\rangle$ plays a central role. A challenge to EPT is to calculate the correlation functions for a distance long enough to compare with field theory. While the applications of EPT-e to 1D fermions and bosons are straightforward, we need yet to see how it works in two dimensions. Finally, the successful calculation of the excitation spectrum indicates that EPT can handle various nanostructures embedded in *correlated* host materials, opening a possible new look at the Kondo effect [21].

[1] D.R.Tilley and J.Tilley, *Superfluidity and Superconductivity* (Adam Hilger LTD, Bristol, 1986).
[2] R.P.Feynman, Phys. Rev. **94**, 262 (1954).
[3] F.D.M.Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[4] I.Affleck, J. Phys. A:Math. Gen. **31**, 4573 (1998).
[5] J.B.Parkinson and J.C.Bonner, Phys. Rev. B **32**, 4703 (1985).
[6] R.Botet and R.Jullien, Phys. Rev. B **27**, 613 (1983).
[7] A.W.Sandvik and D.J.Scalapino, Phys. Rev. B **47**, 12333 (1993).
[8] M.P.Nightingale and H.W.J.Blote, Phys. Rev. B **33**, 659 (1986).
[9] S.R.White and D.A.Huse, Phys. Rev. B **48**, 3844 (1993).
[10] S.R.White, Phys. Rev. B **48**, 10345 (1993).
[11] K.A.Hallberg, P.Horsch, and G.Martinez, Phys. Rev. B **52**, R719 (1995).
[12] J. des Cloiseaux and J.J.Pearson, Phys. Rev. **128**, 2131 (1962).
[13] M.Takahashi, Phys. Rev. B **38**, 5188 (1988).
[14] M.Takahashi, Phys. Rev. Lett. **62**, 2313 (1989).
[15] S.G.Chung, Phys. Lett. A **359**, 707 (2006).
[16] S.G.Chung, Phys. Lett. A **361**, 396 (2007).
[17] S.G.Chung and K.Ueda, Phys. Lett. A **372**, 4845 (2008).
[18] L.Wang and S.G.Chung, unpublished (2009).
[19] M.Karbach, K.Hu, and G.Müller, Computers in Physics **12**, 565 (1998).
[20] S.Ma,   C.Broholm,   D.H.Reich,   B.J.Sternlieb,   and

R.W.Erwin, Phys. Rev. Lett. **69**, 3571 (1992).

[21] A. Otte *et al*, Nature Physics **4**, 847 (2008).